Elves and the acelleration of crystallography

James Holton

Efficient determination of protein crystal structures requires automated X-ray data analysis. I will describe the expert system, Elves, and its use to automatically cary out MAD, SAD and MR structure determinations. All the structure calculations~including indexing, data processing, locating heavy atoms, phasing, model building and refinement--are routinely completed without human intervention. In difficult cases, manual intervention is made easy with an English language interface. The results demonstrate the benefits of automated methods for determining X-ray crystal structures and highlight the importance of intuitive computer interfaces.